Closed form representation for a projection onto infinitely dimensional subspace spanned by Coulomb bound states

O.M. Deryuzhkova[1], **S.B. Levin**[2,3], **S.L. Yakovlev**[2,4]

[1]Department of Physics, Gomel State University, Gomel, Belarus 246019
[2]Department of Computational Physics, St Petersburg University, St Petersburg, Russia 198504
[3]Department of Physics, Stockholm University, Stockholm, Sweden 10691
[4]Department of Physics and Astronomy, California State University at Long Beach, CA 90840

E-mail: `yakovlev@cph10.phys.spbu.ru`

E-mail: `levin@physto.se`

Abstract. The closed form integral representation for the projection onto the subspace spanned by bound states of the two-body Coulomb Hamiltonian is obtained. The projection operator onto the n^2 dimensional subspace corresponding to the n-th eigenvalue in the Coulomb discrete spectrum is also represented as the combination of Laguerre polynomials of n-th and $(n-1)$-th order. The latter allows us to derive an analog of the Christoffel-Darboux summation formula for the Laguerre polynomials. The representations obtained are believed to be helpful in solving the breakup problem in a system of three charged particles where the correct treatment of infinitely many bound states in two body subsystems is one of the most difficult technical problems.

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1. Introduction

The two-body Coulomb problem is perhaps the most famous problem of quantum mechanics formulated on the basis of the Schrödinger wave equation [1]. First solved analytically for the bound states [1], it was then solved for scattering states [2], as well as for the Green's function [3], [4], [5]. The situation is quite different for the systems involving three and more charged particles. There is no analytic solution to the Schrödinger equation in this case and the problem exhibits a great complexity especially if the ionization process is energetically permitted. In this case, the infinitely many open excitation channels are lead to extremely complicated behavior of the wave function, which asymptotically possesses infinitely many terms. Although definite progress has been made in the practical numerical solution of the three charged particles problem above the disintegration threshold [6] by methods avoiding the explicit use of the wave function asymptotics, the theoretical status of the few-body Coulomb problem is still unsatisfactory in many respects. Among the very extensive literature devoted to the few-body Coulomb problem, the following works [7], [8] and [9] refer to the theoretical aspects of the problem.

Recently we have presented a new method of handling the Coulomb potentials in the few-body Hamiltonian with the help of the Coulomb-Fourier transform (CFT) [10]. The method allows us to exclude the long-range Coulomb interaction from the Hamiltonian by a specially constructed unitary transformation. This method was proven useful for repulsive Coulomb interactions. In the case of attraction, the analytic closed form representation for the projections onto the Coulomb bound-states subspace may lead to a substantial simplification of the CFT method machinery. Although the latter was the primary goal, it was found that the representations obtained, being quite general, are not well addressed in the literature, and this has stimulated this publication.

The paper is organized from three sections. After the introduction, in the section two we derive representations for projection operators and consider some particular cases. The third section concludes the paper. Throughout the paper the bold letters, e.g. $\mathbf{r}, \mathbf{r}'$, are used for vectors and not bold for their magnitudes, e.g. $r = |\mathbf{r}|$. The unit vector associated with $\mathbf{r}$ will be denoted by $\hat{\mathbf{r}} = \mathbf{r}/r$.

2. Representations for projections

We consider the infinite dimensional projection operator

$$\mathcal{P}_d = \sum_{n=1}^{\infty} \mathcal{P}_n, \quad \mathcal{P}_{n_1}\mathcal{P}_{n_2} = \delta_{n_1 n_2}\mathcal{P}_{n_1}. \tag{1}$$

The operators $\mathcal{P}_n$ are the orthogonal projections onto the n^2-dimensional subspaces spanned by the two-body Coulomb bound-states $\langle \mathbf{r}|\psi_{nlm}\rangle = \psi_{nlm}(\mathbf{r})$. $\mathcal{P}_n$ have kernels

$$\mathcal{P}_n(\mathbf{r}, \mathbf{r}') = \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \psi_{nlm}(\mathbf{r})\psi^*_{nlm}(\mathbf{r}'), \tag{2}$$

where the normalized Coulomb bound-state wave functions are chosen in the form

$$\psi_{nlm}(\mathbf{r}) = \alpha^{3/2}\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{(n+l)!}}\left(\frac{2\alpha r}{n}\right)^l e^{-\frac{\alpha r}{n}} L_{n-l-1}^{(2l+1)}\left(\frac{2\alpha r}{n}\right) Y_l^m(\hat{\mathbf{r}}). \qquad (3)$$

Here $\alpha = \frac{\mu e^2}{\hbar^2} Z_1 Z_2 > 0$, functions $L_n^{(k)}$ and Y_l^m are the generalized Laguerre polynomials and spherical harmonics as they are defined in [11], respectively. The wave-function $\psi_{nlm}(\mathbf{r})$ obeys the Schrödinger equation

$$(H - E_n)\psi_{nml}(\mathbf{r}) = (-\Delta_{\mathbf{r}} - \frac{2\alpha}{r} - E_n)\psi_{nml}(\mathbf{r}) = 0 \qquad (4)$$

with $E_n = -\alpha^2/n^2$ and n positive integer.

In order to work out the representations for $\mathcal{P}_{d,n}$ we are seeking, let us begin with the standard formula for the projection $\mathcal{P}_n$ as the residue of the Green's function

$$\mathcal{P}_n(\mathbf{r},\mathbf{r}') = \frac{1}{2\pi\mathrm{i}}\oint_{C_{E_n}} \mathcal{G}_c(\mathbf{r},\mathbf{r}',\zeta)d\zeta \qquad (5)$$

with the contour C_{E_n} encircling the point E_n in positive direction in the ζ complex plane. Then, using the Hostler [4] representation for $\mathcal{G}_c(\mathbf{r},\mathbf{r}',\zeta)$

$$\mathcal{G}_c(\mathbf{r},\mathbf{r}',\zeta) = \frac{\Gamma(1-\mathrm{i}\nu)}{4\pi|\mathbf{r}-\mathbf{r}'|}\frac{1}{\mathrm{i}\sqrt{\zeta}}\left(\frac{\partial}{\partial s_+} - \frac{\partial}{\partial s_-}\right) W_{\mathrm{i}\nu,\frac{1}{2}}(-\mathrm{i}\sqrt{\zeta}s_+) M_{\mathrm{i}\nu,\frac{1}{2}}(-\mathrm{i}\sqrt{\zeta}s_-) \qquad (6)$$

where $\nu = \alpha/\sqrt{\zeta}$ and $s_\pm = r + r' \pm |\mathbf{r}-\mathbf{r}'|$ and evaluating the residue, we arrive at the following expression for $\mathcal{P}_n(\mathbf{r},\mathbf{r}')$

$$\mathcal{P}_n(\mathbf{r},\mathbf{r}') = \frac{\alpha^3}{n^4}\frac{e^{-\frac{\alpha}{2n}(s_+ + s_-)}}{\pi(s_+ - s_-)} \qquad (7)$$
$$\times\left[s_+ L_{n-1}\left(\frac{\alpha s_-}{n}\right) L_{n-1}^{(1)}\left(\frac{\alpha s_+}{n}\right) - s_- L_{n-1}^{(1)}\left(\frac{\alpha s_-}{n}\right) L_{n-1}\left(\frac{\alpha s_+}{n}\right)\right].$$

Alternatively, we can transform (7) into the form

$$\mathcal{P}_n(\mathbf{r},\mathbf{r}') = \frac{\alpha^2}{n^2}\frac{e^{-\frac{\alpha}{2n}(s_+ + s_-)}}{\pi(s_+ - s_-)} \qquad (8)$$
$$\times\left\{L_{n-1}\left(\frac{\alpha s_+}{n}\right) L_n\left(\frac{\alpha s_-}{n}\right) - L_n\left(\frac{\alpha s_+}{n}\right) L_{n-1}\left(\frac{\alpha s_-}{n}\right)\right\}.$$

The formulae (7) and (8) are the starting points for representations of this paper.

2.1. Integral representation for projections onto the discrete spectrum subspace

To proceed with formulae (7) and (8), we use the well known expression for Laguerre polynomials [12] in terms of Bessel functions

$$L_{n-1}^{(\beta)}\left(\frac{y}{n}\right) = \frac{n^n}{n!} n^{\beta+1} y^{-\beta/2} e^{y/n}\int_0^\infty dx\, x^{\beta/2-1}\left(xe^{-x}\right)^n J_\beta\left(2\sqrt{xy}\right) \qquad (9)$$

and the following integral representations (3.382.7) [13]

$$\frac{n^n}{n!} = \frac{1}{2\pi}e^n\int_{-\infty}^{\infty}\frac{dy}{(1-\mathrm{i}y)^n}e^{-\mathrm{i}ny}$$

and (6.631.10) [13]

$$\frac{1}{n}e^{\alpha(a+b)/2n} = \int_0^\infty dy\, e^{-ny} I_0\left(\sqrt{2y\alpha(a+b)}\right)$$

where $J_\beta(z)$ and $I_0(z)$ are the Bessel function and the Bessel function of imaginary argument, respectively. Introducing these representations into (7) we arrive at the following integral for $\mathcal{P}_n(\mathbf{r},\mathbf{r}')$

$$\begin{aligned}\mathcal{P}_n(\mathbf{r},\mathbf{r}') &= \frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+ - s_-} \qquad (10)\\ &\times \int_{-\infty}^\infty dy_1 \int_{-\infty}^\infty dy_2 \int_0^\infty dx_3\, I_0\left(\sqrt{2x_3\alpha(s_+ + s_-)}\right)\int_0^\infty \frac{dx_1}{x_1}\int_0^\infty \frac{dx_2}{x_2}\\ &\times \left(\frac{e^{-\mathrm{i}y_1}}{1-\mathrm{i}y_1}\right)^n \left(\frac{e^{-\mathrm{i}y_2}}{1-\mathrm{i}y_2}\right)^n \left(e^{-x_3}\right)^n \left(x_1 e^{-x_1+1}\right)^n \left(x_2 e^{-x_2+1}\right)^n\\ &\times \left[\sqrt{\alpha s_+ x_2}J_0(2\sqrt{\alpha s_- x_1})J_1(2\sqrt{\alpha s_+ x_2}) - \sqrt{\alpha s_- x_2}J_1(2\sqrt{\alpha s_- x_2})J_0(2\sqrt{\alpha s_+ x_1})\right].\end{aligned}$$

By introducing a new five-dimensional variable $X = \{x_1, x_2, x_3, y_1, y_2\}$ and quantities

$$\mathrm{Q} = x_1 e^{-x_1+1} x_2 e^{-x_2+1} e^{-x_3}\frac{e^{-\mathrm{i}y_1}}{1-\mathrm{i}y_1}\frac{e^{-\mathrm{i}y_2}}{1-\mathrm{i}y_2},$$

$$\begin{aligned}B(X,\alpha,s_+,s_-) &= I_0\left(\sqrt{2x_3\alpha(s_+ + s_-)}\right)\\ &\times \left[\sqrt{\alpha s_+ x_2}J_0(2\sqrt{\alpha s_- x_1})J_1(2\sqrt{\alpha s_+ x_2}) - \sqrt{\alpha s_- x_2}J_1(2\sqrt{\alpha s_- x_2})J_0(2\sqrt{\alpha s_+ x_1})\right]\end{aligned}$$

we rewrite the latter formula in the compact form

$$\mathcal{P}_n(\mathbf{r},\mathbf{r}') = \frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+ - s_-}\int\limits_\Omega \frac{dX}{x_1 x_2}\mathrm{Q}^n B(X,\alpha,s_+,s_-). \qquad (11)$$

The integration domain Ω is defined as

$$\Omega = \{X : 0 \le x_i < \infty,\ i = 1,2,3,\ -\infty < y_k < \infty,\ k = 1,2\}. \qquad (12)$$

Let us notice that the quantity $|\mathrm{Q}|$ is bounded on Ω with the only maximum (such that $|\mathrm{Q}| = 1$) at the point $X_0 = \{1,1,0,0,0\}$, hence everywhere except X_0 the inequality $|\mathrm{Q}| < 1$ holds true.

Before computing the infinite sum (1) let us consider the operator

$$\mathcal{P}_{N_1}^{N_2} = \sum_{n=N_1}^{N_2}\mathcal{P}_n. \qquad (13)$$

The kernel of the operator $\mathcal{P}_{N_1}^{N_2}$ can easily be computed by using the formula (11) for $\mathcal{P}_n$ and evaluating of the sum of the geometric progression of Q^n terms under the integral which yield

$$\mathcal{P}_{N_1}^{N_2}(\mathbf{r},\mathbf{r}') = P_{N_1}^{N_2}(\mathbf{r},\mathbf{r}',\Omega) \equiv \frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+ - s_-} \qquad (14)$$

$$\times \int\limits_{\Omega} \frac{dX}{x_1 x_2} \frac{\mathrm{Q}^{N_1}(1-\mathrm{Q}^{N_2-N_1+1})}{1-\mathrm{Q}} B(X,\alpha,s_+,s_-).$$

Now we are ready to evaluate the limit of $P_{N_1}^{N_2}(\mathbf{r},\mathbf{r}',\Omega)$ as $N_2 \to \infty$ keeping N_1 finite. Let us notice that the integral (14) converges uniformly at any N_2 and hence for any positive ϵ we can find $\delta > 0$ such that

$$|P_{N_1}^{N_2}(\mathbf{r},\mathbf{r}',\Omega(X_0,\delta))| < \epsilon \tag{15}$$

where $\Omega(X_0,\delta)$ is a neighborhood of the point X_0 in which the quantity Q reaches its maximum, i.e.

$$\Omega(X_0,\delta) = \{X \in \Omega : |X - X_0| < \delta\}. \tag{16}$$

On the rest of the integration domain $\overline{\Omega}(X_0,\delta) \equiv \Omega \backslash \Omega(X_0,\delta)$ the inequality $|\mathrm{Q}| < 1$ holds true and we can take the limit

$$P_{N_1}(\mathbf{r},\mathbf{r}',\overline{\Omega}(X_0,\delta)) = \lim_{N_2\to\infty} P_{N_1}^{N_2}(\mathbf{r},\mathbf{r}',\overline{\Omega}(X_0,\delta)) = \tag{17}$$

$$\frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+-s_-}\int\limits_{\overline{\Omega}(X_0,\delta)} \frac{dX}{x_1x_2}\frac{\mathrm{Q}^{N_1}}{1-\mathrm{Q}} B(X,\alpha,s_+,s_-). \tag{18}$$

For the integral (18) the limit $\delta \to 0$ is permitted, so that due to the arbitrariness of ϵ we get

$$\mathcal{P}_{N_1}(\mathbf{r},\mathbf{r}') = \lim_{\delta\to 0} P_{N_1}(\mathbf{r},\mathbf{r}',\overline{\Omega}(X_0,\delta)) = \tag{19}$$

$$\frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+-s_-}\int\limits_{\Omega} \frac{dX}{x_1x_2}\frac{\mathrm{Q}^{N_1}}{1-\mathrm{Q}} B(X,\alpha,s_+,s_-).$$

Now by setting $N_1 = 1$ we arrive at the final result for the projection $\mathcal{P}_d$

$$\mathcal{P}_d(\mathbf{r},\mathbf{r}') = \frac{1}{(2\pi)^3}\frac{2\alpha^2}{s_+-s_-}\int\limits_{\Omega} \frac{dX}{x_1x_2}\frac{\mathrm{Q}}{1-\mathrm{Q}} B(X,\alpha,s_+,s_-). \tag{20}$$

The formulae (19) and (20) are the main results of this subsection.

2.2. Some particular cases

In this subsection we consider a particular case of the integral representation (8) which leads to an analog of the Christoffel-Darboux formula (22.12.1) [11] applied to Laguerre polynomials. We also evaluate the asymptotics of the projections kernel $\mathcal{P}_n(\mathbf{r},\mathbf{r}')$ in the special case when $n \gg \alpha(r+r')$ with the help of representation (7).

It is worthwhile to notice that the formulae (7,8) in the particular case when $n = 1, 2$

$$\mathcal{P}_1(\mathbf{r},\mathbf{r}') = \frac{\alpha^3}{\pi} e^{-\alpha(r+r')}, \tag{21}$$

$$\mathcal{P}_2(\mathbf{r},\mathbf{r}') = \frac{\alpha^3}{32\pi} e^{-\frac{\alpha}{2}(r+r')} \left[4 - 2\alpha(r+r') + \alpha^2 rr(1+\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}')\right] \tag{22}$$

give essentially the same results which can be computed directly from the conventional representation (2,3). Let us now consider the case of arbitrary n. From (2,3) and (8) we get

$$\frac{L_{n-1}(\frac{\alpha s_+}{n})L_n(\frac{\alpha s_-}{n}) - L_n(\frac{\alpha s_+}{n})L_{n-1}(\frac{\alpha s_-}{n})}{\frac{\alpha}{n}(s_+ - s_-)} = \tag{23}$$

$$\frac{1}{n}\sum_{l=0}^{n-1}\left(\frac{2\alpha r}{n}\frac{2\alpha r'}{n}\right)^l \frac{(n-l-1)!}{(n+l)!} L_{n-l-1}^{(2l+1)}\left(\frac{2\alpha r}{n}\right) L_{n-l-1}^{(2l+1)}\left(\frac{2\alpha r'}{n}\right)(2l+1)P_l(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}').$$

Taking a particular case $\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}' = 1$, setting $(2\alpha r)/n = x$, $(2\alpha r')/n = y$ and changing the summation variable in such a way $l = n - m - 1$ we get

$$\frac{L_{n-1}(x)L_n(y) - L_n(x)L_{n-1}(y)}{x-y} = \tag{24}$$

$$\frac{1}{n}\sum_{m=0}^{n-1}(xy)^{n-m-1}\frac{m!(2(n-m)-1)}{(2n-m-1)!}L_m^{(2(n-m)-1)}(x)L_m^{(2(n-m)-1)}(y).$$

This formula if compared to the Christoffel-Darboux summation formula for Laguerre polynomials (22.12.1) [11]

$$\frac{L_{n-1}(x)L_n(y) - L_n(x)L_{n-1}(y)}{x-y} = \frac{1}{n}\sum_{m=0}^{n-1}L_m(x)L_m(y) \tag{25}$$

yields the following interesting identity

$$\sum_{m=0}^{n-1}L_m(x)L_m(y) = \tag{26}$$

$$\sum_{m=0}^{n-1}(xy)^{n-m-1}\frac{m!(2(n-m)-1)}{(2n-m-1)!}L_m^{(2(n-m)-1)}(x)L_m^{(2(n-m)-1)}(y).$$

As the last special case we consider the behavior of the projection $\mathcal{P}_n$ for large value of the principal quantum number n. Let us use again the representation (9) which we rewrite in the form

$$L_{n-1}^{(\beta)}(y/n) = \frac{n^n}{n!}n^{\beta+1}y^{-1/2\beta}e^{y/n}F^\beta(n,y)$$

where $F^\beta(n,y)$ stands for the integral

$$F^\beta(n,y) = \int_0^\infty dx\, x^{\beta/2-1}e^{-n(x-\log x)}J_\beta(2\sqrt{xy})$$

and introduce it into the formula (7) for Laguerre polynomials. If $n \gg \alpha(r+r')$ then the only critical factor under the respective integrals $F^\beta(n,\alpha s_\pm)$ is $e^{-n(x-\log x)}$ with the only critical point $x_0 = 1$. Evaluating the the integrals $F^\beta(n,\alpha s_\pm)$ as $n\to\infty$ by the Laplace method we get for the projections $\mathcal{P}_n(\mathbf{r},\mathbf{r}')$ the following asymptotics

$$\mathcal{P}_n(\mathbf{r},\mathbf{r}') \propto \frac{\alpha^{5/2}}{\pi n^3(s_+ - s_-)}[\sqrt{s_+}J_0(2\sqrt{\alpha s_-})J_1(2\sqrt{\alpha s_+}) - \sqrt{s_-}J_1(2\sqrt{\alpha s_-})J_0(2\sqrt{\alpha s_+})].$$

3. Conclusion

The closed form representations are obtained for projections onto the n^2-dimensional subspace spanned by bound-state eigenfunctions of the Coulomb Hamiltonian corresponding to the principal quantum number n as well as for the projection onto the subspace spanned by all Coulomb bound-states. These representations can be useful for solving the few body scattering problem in a system of charged particles for energies above the three body disintegration thresholds. The asymptotics computed above for the projections $\mathcal{P}_n$ as $n \to \infty$ may lead to drastic simplifications in calculating different Coulomb matrix elements between states which are spatially well confined. The analog of the Christoffel-Darboux summation formula for Laguerre polynomials which is derived as a particular case of the representations for the Coulomb projections can be useful for the theory of classical orthogonal polynomials.

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References

[1] Schrödinger E 1926 *Ann. der Phys.* **79** 361
[2] Yost F, Weeler J and Breit G 1936 *Phys. Rev.* **49** 174
[3] Wichmann E H, Woo C H 1961 *J. Math. Phys.* **2** 178
[4] Hostler L 1962 *Bull. Am. Phys. Soc.* **7** 609; Hostler L, Pratt R 1963 *Phys. Rev. Lett.* **10** 469; Hostler L 1964 *J. Math. Phys.* **5** 591
[5] Schwinger J 1964 *J. Math. Phys.* **5** 1606
[6] Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 *Science* **286** 2474; Baertschy M, Rescigno T N and McCurdy C W 2001 *Phys. Rev.* A **64** 022709; Bray I (2002) *Phys. Rev. Lett.* **89** 273201
[7] Rudge M R H 1968 *Rev. Mod. Phys.* **40** 564
[8] Peterkop R K *Theory of Ionization of Atoms by Electron-Impact* (Colorado Associated University Press, Boulder, 1977)
[9] Faddeev L D and Merkuriev S P *Quantum Scattering Theory for Several Particle Systems* (Kluwer, Dordrecht, 1993)
[10] Alt E O, Levin S B and Yakovlev S L 2004 *Phys. Rev.* C **69** 034002
[11] *Handbook of Mathematical Functions* edited by Abramovitz M and Stegun I A (Dover, New York, 1986)
[12] Bateman H *Higher Transcendental Functions* (McGraw-Hill Book Company, New York, 1953)
[13] Gradshteyn I S and Ryzhik I M *Table of Integrals, Series, and Products* (Academic Press, San Diego, 1980)